# Adaptive Low Mach Number Combustion

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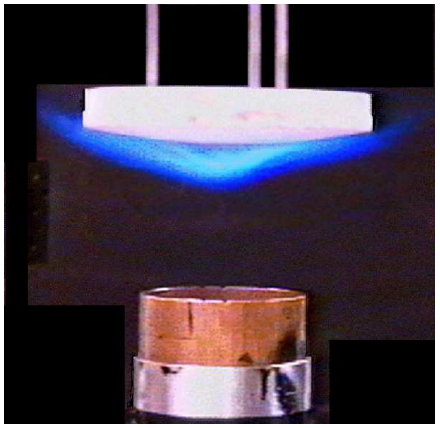
# Lean Premixed Turbulent Combustion

Rod-stabilized V-flame

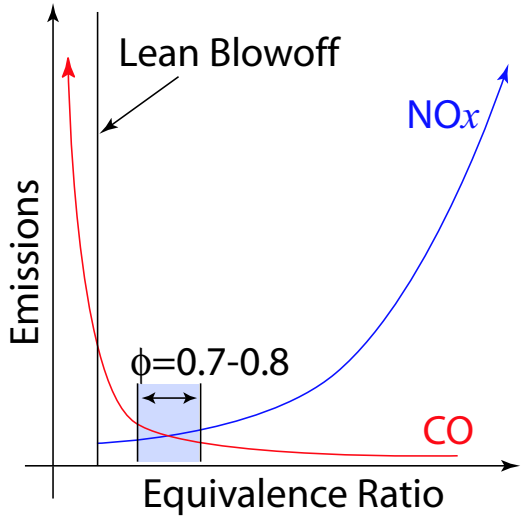
4-jet Low-swirl burner (LSB)



Stagnation flame

We would like to study these types of flame computationally

- Potential for efficient, low-emission power systems
- Design issues because of flame instabilities
- Limitations of theory and experiment




Questions to address

- Basic flame dynamics
- Turbulence / chemistry interaction

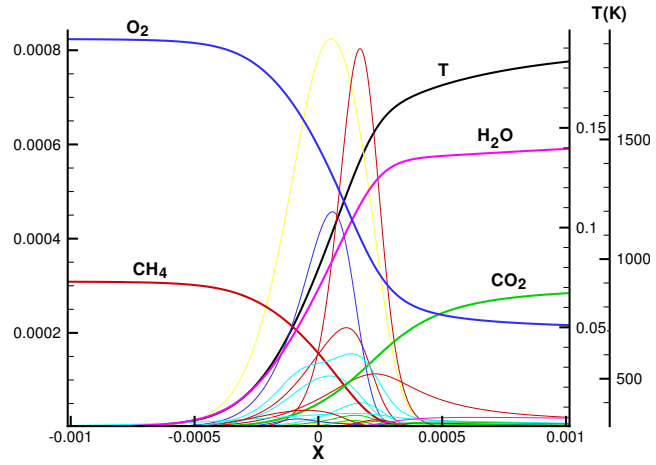
# Premixed flames

Basic methane combustion

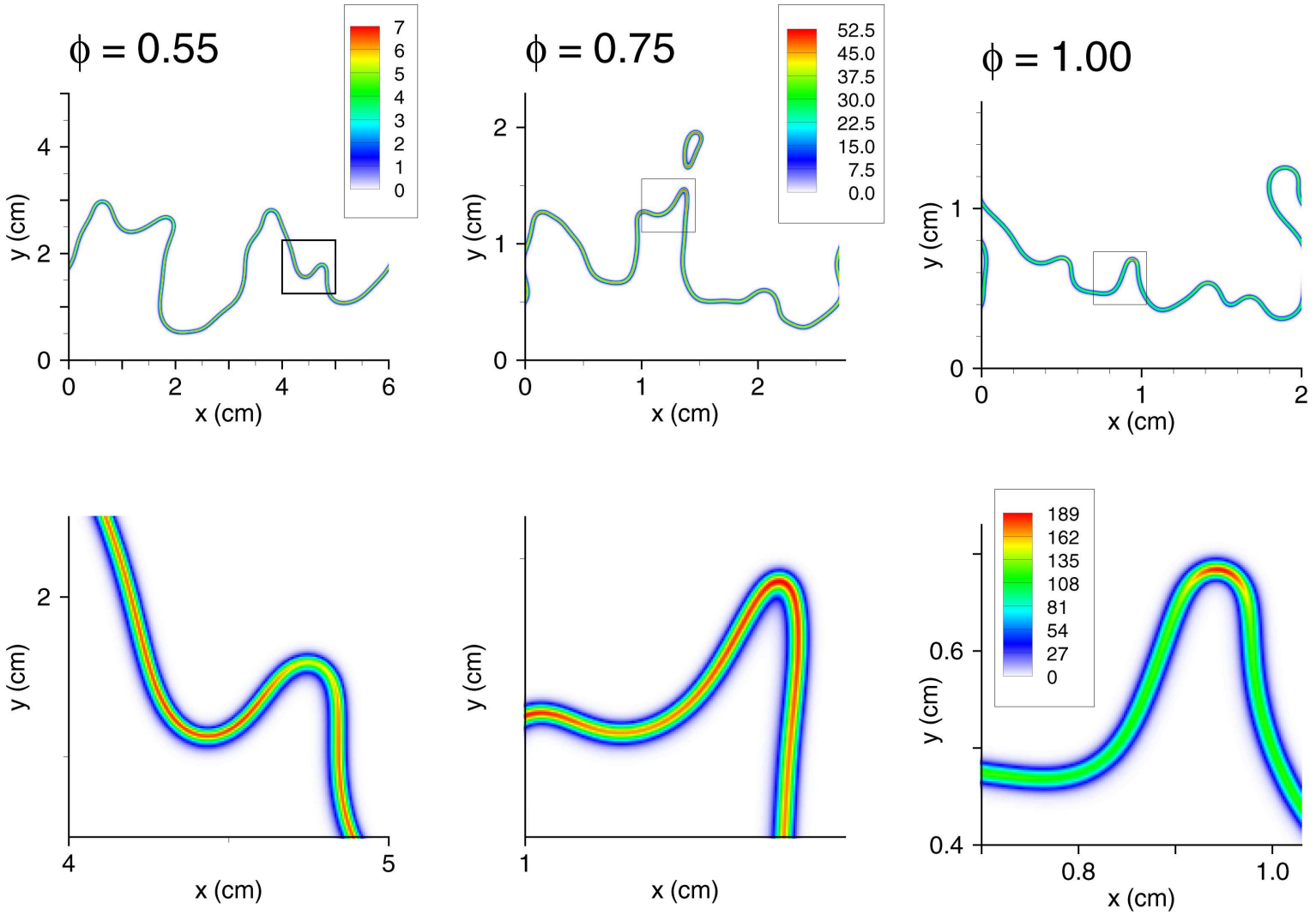
- $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + \text{heat}$
- Multiple intermediate species, many reactions
- Initial reactions form radicals (chain initiating)
- Additional reactions multiply radical pool (chain branching)
- Radicals combine to form stable products (chain terminating)
- Requires heat to initiate reactions

How does this work in a premixed flame?

- Released heat sustains reactions
- Heat and radicals formed "inside" the flame diffuse into fuel to initiate reactions
- Balance of diffusion and reaction

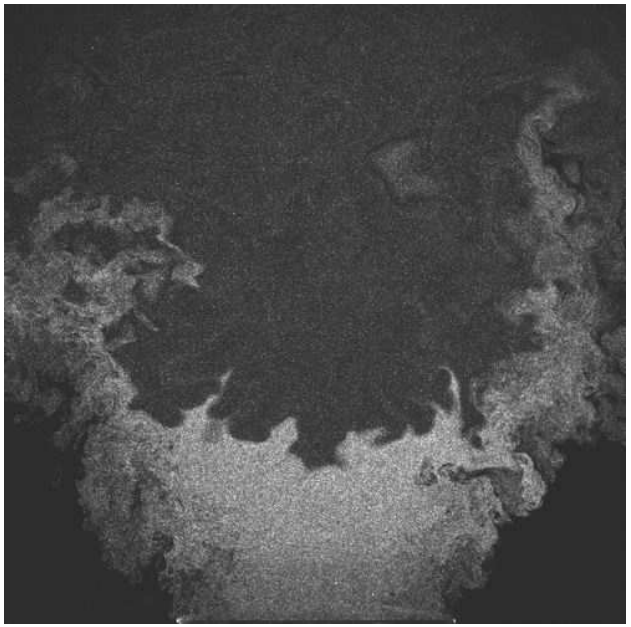


# Effect of chemistry on flame



# Relevant Scales

- Domain: $O(10)$ cm
- Mean Flow: $O(10^3)$ cm/s
- Acoustic Speed: $O(10^5)$ cm / s
- Flame thickness: $\delta_T = O(10^{-1})$ cm
- Integral scale: $O(10^0 - 10^{-1})$ cm
- Kolmogorov scales: $O(10^{-2})$ cm
- Time scale: 0.1 - 1.0 sec
- Chemical scale: $O(10^{-6})$ sec or less



# Objective

What are the requirements for simulating these types of flames

1. No explicit model for turbulence, or turbulence/chemistry interactions
2. Detailed chemistry based on fundamental reactions, detailed diffusion
3. Incorporate "sufficient" range of space and time scales

Wide range of scales + Multi-physics

- Fluid mechanics
- Chemistry
- Multicomponent species transport
- Thermal radiation and conduction

Standard approach – compressible flow formulation

- $O(10)$ species; $O(10^2)$ reactions
- $O(10^9)$ zones
- $O(10^6)$ time steps

This approach is not tractable with existing hardware

# Approach

Exploit natural separations of scale to build effective simulation methodology

Observation:

- Laboratory turbulent flames are low Mach number
- Regions requiring high-resolution are localized in space

Our approach:

- Low Mach number formulation
  - Eliminate acoustic time-step restriction while retaining compressibility effects due to heat release
  - Conserve species and enthalpy
- Adaptive mesh refinement
  - Localize mesh where needed
  - Complexity from synchronization of elliptic solves
- Parallel architectures
  - Distributed memory implementation using BoxLib framework
  - Dynamic load balancing
  - Heterogeneous work load

# Low Mach Number Combustion

Low Mach number model, $M = U/c \ll 1$ (Rehm & Baum 1978, Majda & Sethian 1985)

Start with the compressible Navier-Stokes equations for multicomponent reacting flow, and expand in the Mach number, $M = U/c$.

Asymptotic analysis shows that:

$$p(\vec{x}, t) = p_0(t) + \pi(\vec{x}, t) \quad \text{where} \quad \pi/p_0 \sim \mathcal{O}(M^2)$$

- $p_0$ does not affect local dynamics, $\pi$ does not affect thermodynamics
- For open containers $p_0$ is constant
- Acoustic waves analytically removed (or, have been "relaxed" away)

# Low Mach number equations

$$\textbf{Momentum} \quad \rho\frac{DU}{Dt} = -\nabla\pi + \nabla\cdot\left[\mu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot U\right)\right]$$

$$\textbf{Species} \quad \frac{\partial(\rho Y_m)}{\partial t} + \nabla\cdot(\rho U Y_m) = \nabla\cdot(\rho D_m \nabla Y_m) + \dot{\omega}_m$$

$$\textbf{Mass} \quad \frac{\partial\rho}{\partial t} + \nabla\cdot(\rho U) = 0$$

$$\textbf{Energy} \quad \frac{\partial\rho h}{\partial t} + \nabla\cdot\left(\rho h\vec{U}\right) = \nabla\cdot(\lambda\nabla T) + \sum_m \nabla\cdot(\rho h_m D_m \nabla Y_m)$$

Equation of state $p_0 = \rho\mathcal{R}T\sum_m \frac{Y_m}{W_m}$

System contains four evolution equations for $U, Y_m, \rho, h$, with a constraint given by the EOS.

# Constraint for reacting flows

Low Mach number system is a system of PDE's evolving subject to a constraint; differential algebraic equation (DAE)

Standard approach is to differentiate constraint to obtain IVP

Here, we differentiate the EOS along particle paths and use the evolution equations for $\rho$ and $T$ to define a constraint on the velocity:

$$\begin{aligned}
\nabla \cdot U = \frac{1}{\rho}\frac{D\rho}{Dt} &= -\frac{1}{T}\frac{DT}{Dt} - \frac{\mathcal{R}}{R}\sum_m \frac{1}{W_m}\frac{DY_m}{Dt} \\
&= \frac{1}{\rho c_p T}\left(\nabla\cdot(\lambda\nabla T) + \sum_m \rho D_m \nabla Y_m \cdot \nabla h_m\right) \; + \\
&\quad \frac{1}{\rho}\sum_m \frac{W}{W_m}\nabla(D_m\rho\nabla Y_m) \; + \; \frac{1}{\rho}\sum_m\left(\frac{W}{W_m} - \frac{h_m(T)}{c_pT}\right)\dot{\omega_m} \\
&\equiv S
\end{aligned}$$

# Incompressible Navier Stokes Equations

For iso-thermal, single fluid systems this analysis leads to the incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

How do we develop efficient integration schemes for this type of constrained evolution system?

Vector field decomposition

$$V = U_d + \nabla \phi$$

where $\nabla \cdot U_d = 0$

and

$$\int U \cdot \nabla \phi dx = 0$$

We can define a projection $\mathbf{P}$

$$\mathbf{P} = I - \nabla(\Delta^{-1})\nabla\cdot$$

such that $U_d = \mathbf{P}V$

Solve

$$-\Delta \phi = \nabla \cdot V$$

# Projection method

Incompressible Navier Stokes equations

$$U_t + U \cdot \nabla U + \nabla \pi = \mu \Delta U$$

$$\nabla \cdot U = 0$$

## Projection method

Advection step

$$\frac{U^* - U^n}{\Delta t} + U \cdot \nabla U = {}^1\!/_2 \mu \Delta (U^* + U_n) - \nabla \pi^{n-{}^1\!/_2}$$

Projection step

$$U^{n+1} = \mathbf{P} U^*$$

Recasts system as initial value problem

$$U_t + \mathbf{P}(U \cdot \nabla U - \mu \Delta U) = 0$$

# Combustion system

The form of the system we use is then

$$\frac{\partial U}{\partial t} + (U \cdot \nabla)U + \frac{1}{\rho}\nabla\pi = \frac{1}{\rho}\nabla \cdot \tau$$

$$\frac{\partial(\rho Y_m)}{\partial t} + \nabla \cdot (\rho U Y_m) = D_Y + R_Y$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0$$

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho U h) = D_h$$

$$\nabla \cdot U = S$$

# LMC approaches

How can this approach be generalized to low Mach number reacting flows?

- Finite amplitude density variations
- Compressiblility effects

Proposed extensions of the projection method fall into two basic classes:

Constant coefficient "projection"

- McMurtry, Riley, Metcalfe, AIAA J., 1986.
- Rutland & Fertziger, C&F, 1991.
- Zhang and Rutland, C&F, 1995.
- Cook and Riley, JCP, 1996.
- Najm, Trans. Phen. in Comb., 1996
- Najm & Wyckoff, C&F, 1997.
- Quian, Tryggvason & Law, JCP 1998.
- Najm, Knio & Wyckoff, JCP, 1998.

Variable coefficient projection

- Bell & Marcus, JCP, 1992.
- Lai, Bell, Colella, 11th AIAA CFD, 1993.
- Pember et al., Comb. Inst. WSS, 1995.
- Pember et al., Trans. Phen. Comb., 1996.
- Pember et al., CST, 1998.
- Schneider et al., JCP, 1999.
- Day & Bell, CTM, 2000.
- Nicoud, JCP, 2000.

# Variable coefficient projection

Generalized vector field decomposition

$$V = U_d + \frac{1}{\rho}\nabla\phi$$

where $\nabla \cdot U_d = 0$ and $U_d \cdot n = 0$ on the boundary

Then $U_d$ and $\frac{1}{\rho}\nabla\phi$ are orthogonal in a density weighted space.

$$\int \frac{1}{\rho}\nabla\phi \cdot U \ \rho \ dx = 0$$

Defines a projection $\mathbf{P}_\rho = I - \frac{1}{\rho}\nabla((\nabla \cdot \frac{1}{\rho}\nabla)^{-1})\nabla\cdot$ such that $\mathbf{P}_\rho V = U_d$.

$\mathbf{P}_\rho$ is idempotent and $||\mathbf{P}_\rho|| = 1$

# Variable coefficient projection method

We can use this projection to define a projection scheme for the variable density system

$$\rho_t + \nabla \cdot \rho u = 0$$

$$U_t + U \cdot \nabla U + \frac{1}{\rho} \nabla \pi = 0$$

$$\nabla \cdot U = 0$$

Advection step

$$\rho^{n+1} = \rho^n - \Delta t \nabla \cdot \rho U$$

$$U^* = U^n - \Delta t \, U \nabla \cdot U - \frac{1}{\rho} \nabla \pi^{n-1/2}$$

Projection step

$$U^{n+1} = \mathbf{P}_\rho U_d$$

Recasts system as initial value problem

$$U_t + \mathbf{P}_\rho (U \cdot \nabla U) = 0$$

# Inhomogeneous constraints

We can use the variable-$\rho$ projection to define a projection scheme for inhomogeneous constraints

$$U_t + U \cdot \nabla U + \frac{1}{\rho} \nabla \pi = \tau$$

$$\nabla \cdot U = S$$

Advection step

$$U^* = U^n - \Delta t \, U \nabla \cdot U = \Delta t \, \tau - \frac{1}{\rho} \nabla \pi^{n-1/2}$$

Projection step

$$U = U_d + \nabla \xi$$

where

$$\nabla \cdot \nabla \xi = S$$

$$U^{n+1} = \mathbf{P}_\rho (U^* - \nabla \xi) + \nabla \xi$$

# 2nd Order Fractional Step Scheme

First Step:

Construct an intermediate velocity field $U^*$:

$$\frac{U^* - U^n}{\Delta t} = -[U^{ADV} \cdot \nabla U]^{n+\frac{1}{2}} - \frac{1}{\rho^{n+\frac{1}{2}}} \nabla \pi^{n-\frac{1}{2}} + \frac{1}{\rho^{n+\frac{1}{2}}} \nabla \cdot \frac{\tau^n + \tau^*}{2}$$

and advance species concentrations and enthalpy

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} = -\nabla \cdot (\rho U^{ADV})^{n+\frac{1}{2}}$$

$$\frac{\rho^{n+1}\chi^{n+1} - \rho^n \chi^n}{\Delta t} + \nabla \cdot (\rho U^{ADV} \chi)^{n+\frac{1}{2}} = D_\chi + R_\chi \quad for\ \chi = h, Y_m$$

# Enforce the constraint

Use the updated values to compute $S^{n+1}$

Decompose $\vec{U}^{n+1,*}$ to extract the component satisfying the divergence constraint.

This decomposition is achieved by solving

$$\nabla \cdot \left( \frac{1}{\rho} \nabla \phi \right) = \nabla \cdot \vec{U}^{n+1,*} - S^{n+1}$$

for $\phi$, and setting

$$\pi^{n+1/2} = \pi^{n-1/2} + \phi$$

and

$$\vec{U}^{n+1} = \vec{U}^{n+1,*} - \frac{1}{\rho} \nabla \phi$$

Exploits linearity to represent the compressible component of the velocity

# Properties of the methodology

Overall operator-split projection formulation is $2^{nd}$-order accurate in space and time.

Godunov-type discretization of advection terms provides a robust $2^{nd}$-order accurate treatment of advective transport.

Formulation conserves species, mass and energy.

Equation of state is only approximately satisfied

$$p_o \neq \rho RT \sum_m \frac{Y_m}{W_m}$$

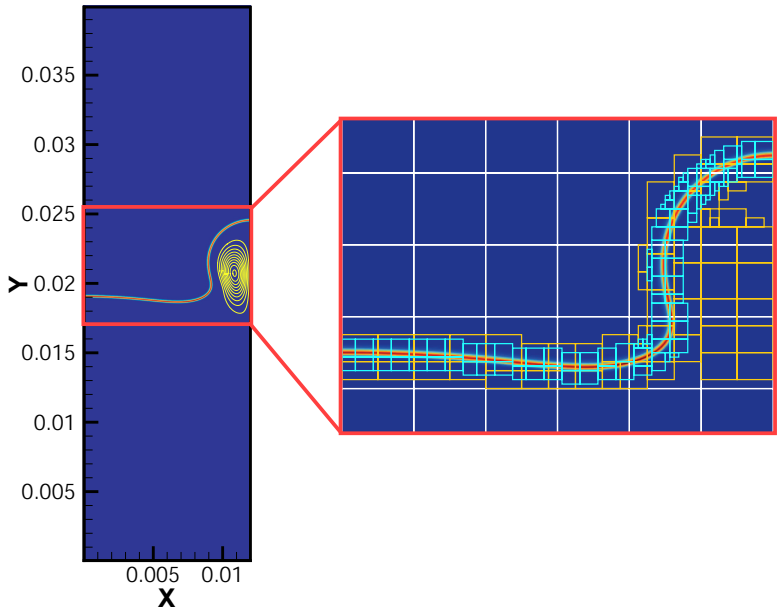
but modified constraint minimizes drift from equation of state.

# AMR - Grid Structure

Block-structured hierarchical grids

Each grid patch (2D or 3D)

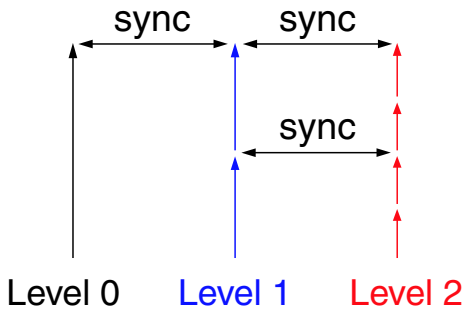
- Logically structured, rectangular
- Refined in space and time by evenly dividing coarse grid cells
- Dynamically created/destroyed to track time-dependent features




2D adaptive grid hierarchy

Subcycling:

- Advance level $\ell$, then
  - Advance level $\ell + 1$
    level $\ell$ supplies boundary data
  - Synchronize levels $\ell$ and $\ell + 1$




*Preserves properties of single-grid algorithm*

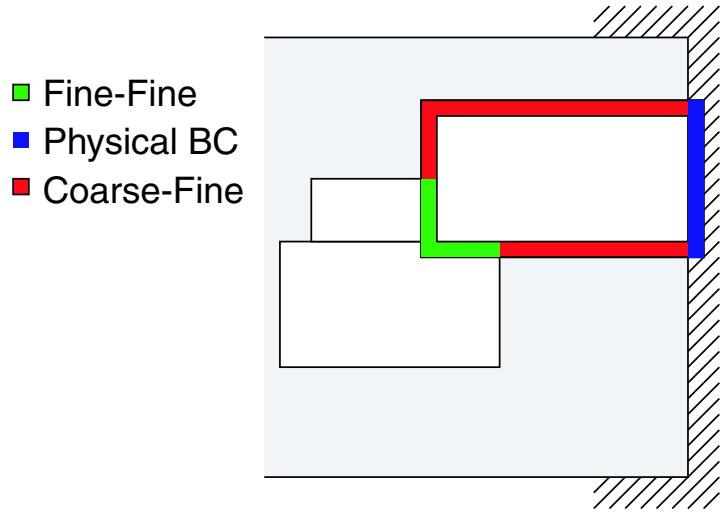
# AMR Synchronization

Coarse grid supplies Dirichlet data as boundary conditions for the fine grids.

Errors take the form of flux mismatches at the coarse/fine interface.

Design Principles:

- Define what is meant by the solution on the grid hierarchy.
- Identify the errors that result from solving the equations on each level of the hierarchy “independently” (motivated by subcycling in time).
- Solve correction equation(s) to “fix” the solution.
- For subcycling, average the correction in time.



# Synchronization Corrections

Syncrhonization corrects mismatch in fluxes at coarse / fine boundaries
Correction equations match the structure of the process they are correcting.

- For explicit discretizations of **hyperbolic** PDE's the correction is an explicit flux correction localized at the coarse/fine interface.
- For an **elliptic** equation (e.g., the projection) the source is localized on the coarse/fine interface but an elliptic equation is solved to distribute the correction through the domain. Discrete analog of a layer potential problem.
- For Crank-Nicolson discretization of **parabolic** PDE's, the correction source is localized on the coarse/fine interface but the correction equation diffuses the correction throughout the domain.

Performing corrections for each step of the low Mach number projection algorithm guarantees that the adaptive algorithm preserves the properties of the single grid scheme.

# Dynamic Load-Balancing

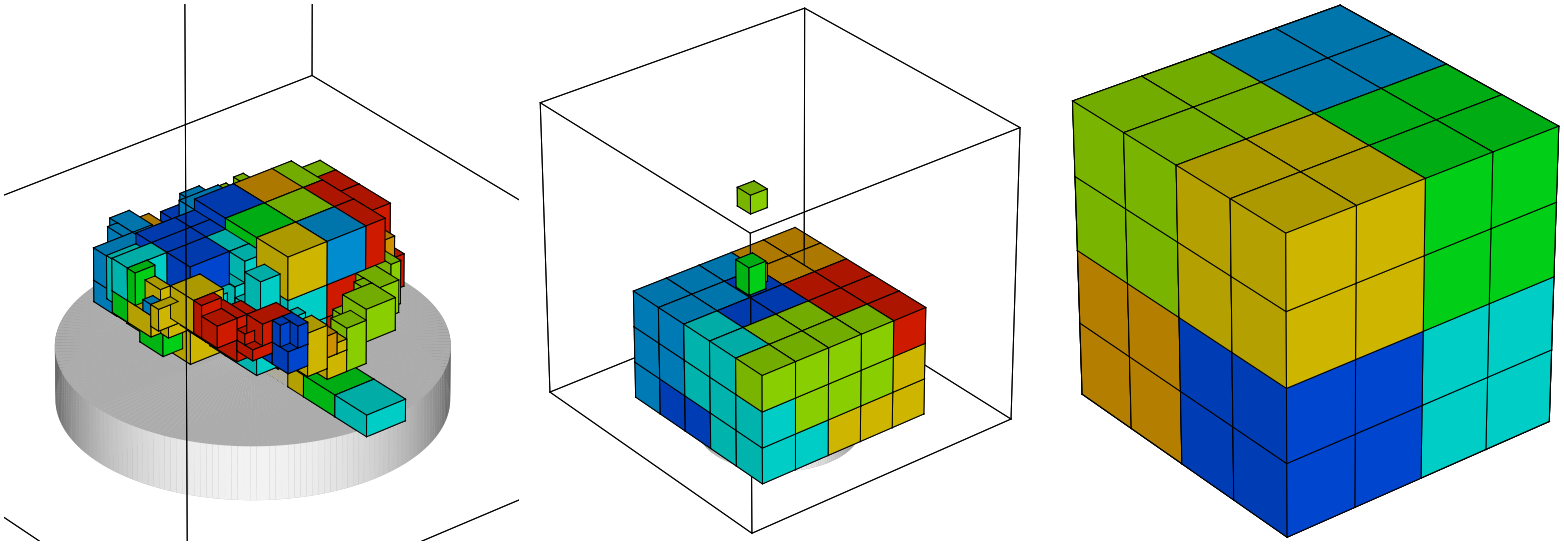
Approach: Estimate work per grid, distribute using heuristic KNAPSACK algorithm

Cells/grid often a good work estimate, but chemical kinetics may be highly variable

- Monitor chemistry integration work
- Distribute chemistry work based on this work estimate

Parallel Communication: AMR data communication patterns are complex

- Easy: distribute grids at a single level, minimize off-processor communication
- Hard: Incorporate coarse-fine interpolation (also, “recursive” interpolation)



Level 2 Level 1 Level 0

# Model problems

## 2-D Vortex flame interactions

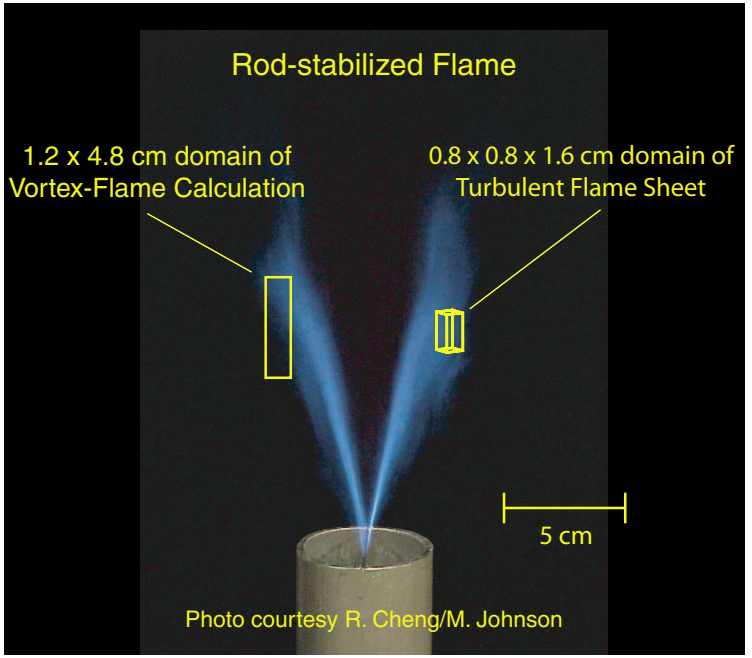
($28^{th}$ International Combustion Sympsium, 2000)

- $1.2 \times 4.8$ mm domain
- 32 species, 177 reactions

## 3-D Turbulent flame sheet

($29^{th}$ International Combustion Sympsium, 2002)

- $.8 \times .8 \times 1.6$ cm domain
- 20 species, 84 reactions

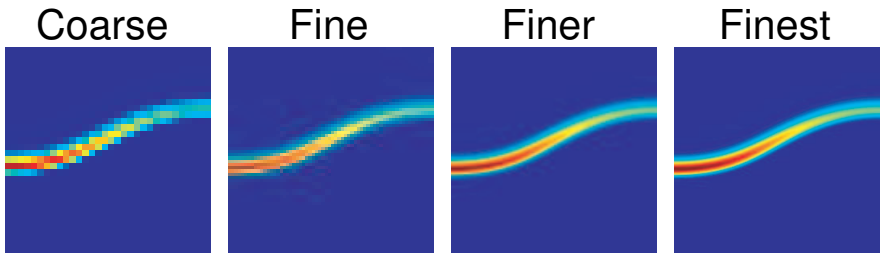


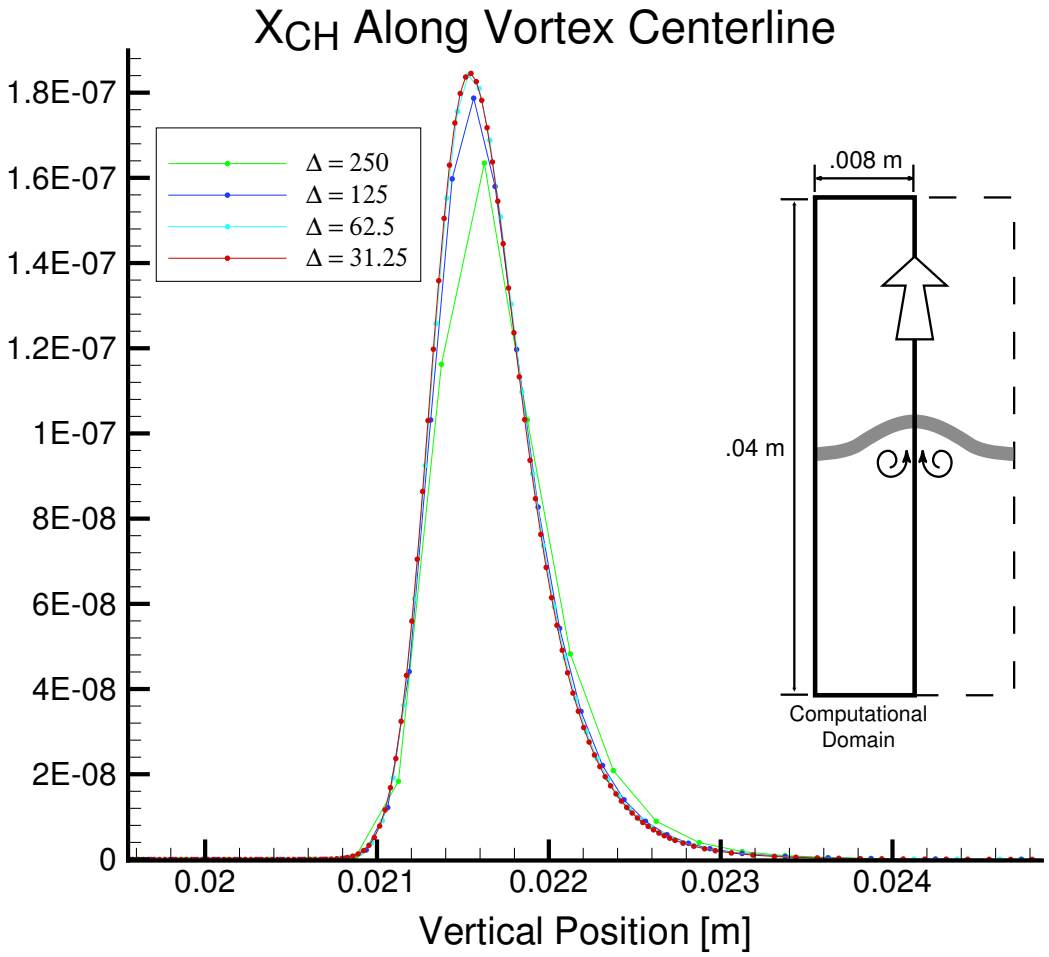

## Laboratory-scale V-flame

($19^{th}$ International Colloquium on the Dynamics of Explosions and Reactive Systems, 2003)

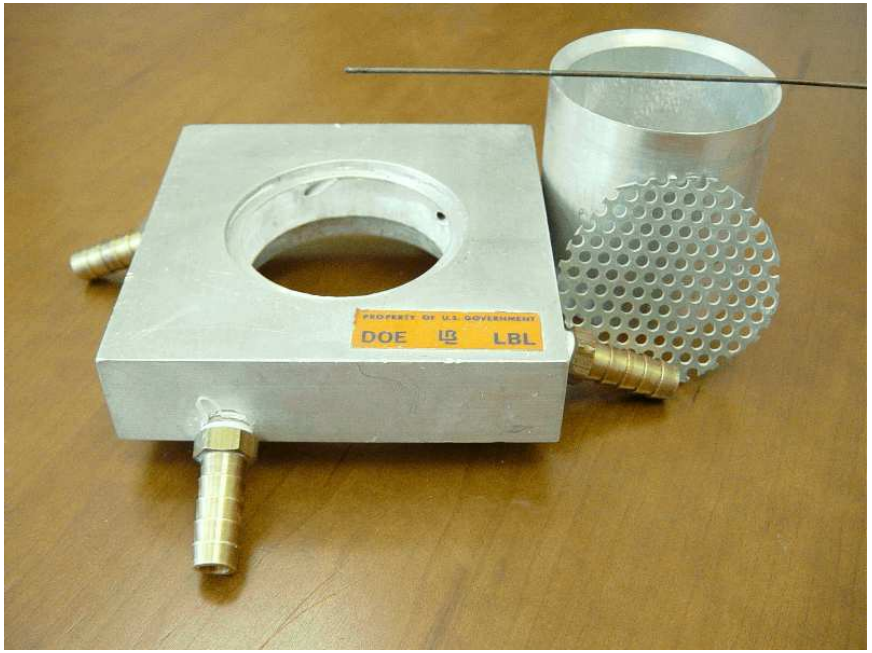
- $12 \times 12 \times 12$ cm domain
- 20 species, 84 reactions

# Convergence Behavior

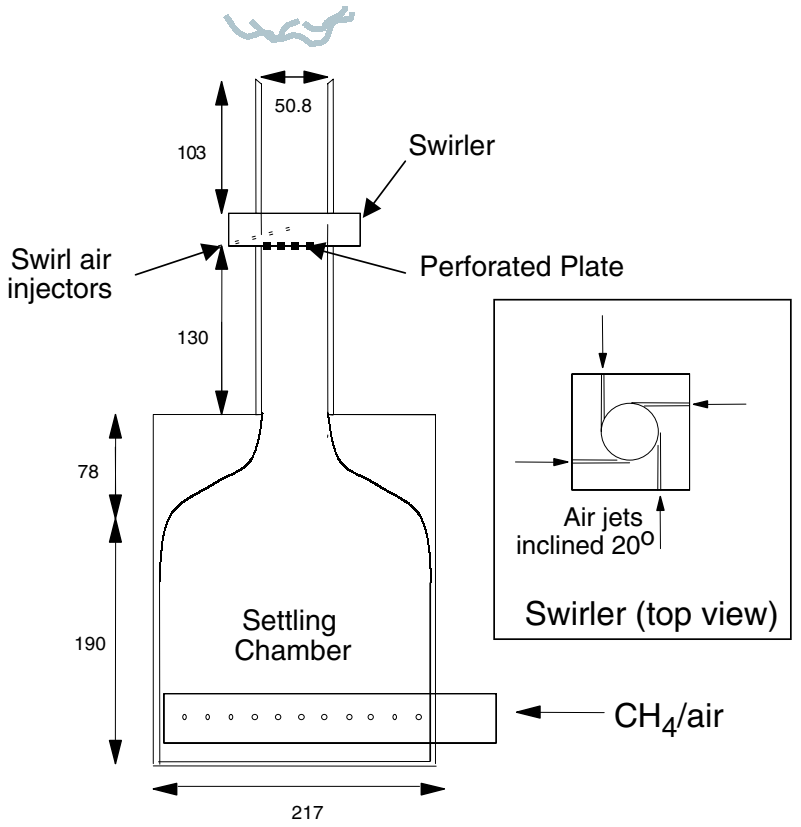


# Configuration




Burner assembly

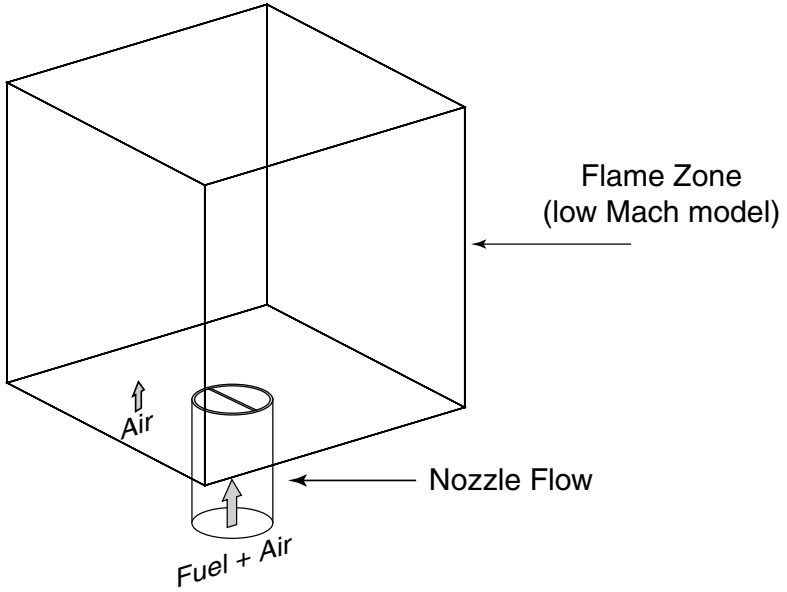



Experiment schematic

- V-flame ($\dot{m}_{air} \equiv 0$): rod $\sim$ 1 mm
- Turbulence plate: 3 mm holes on 4.8 mm center

# V-flame Setup

Strategy - Treat nozzle exit as inflow boundary condition for combustion simulation




- 12cm x 12cm x 12cm domain
- DRM-19: 20 species, 84 reactions
- Mixture model for differential diffusion

Inflow characteristics

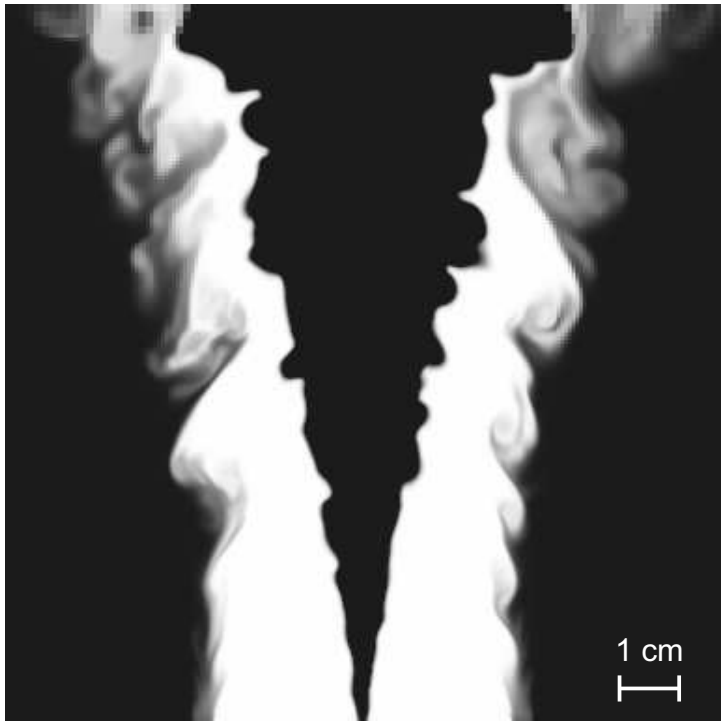
- Mean flow
  - 3 m/s mean inflow
  - Boundary layer profile at edge
  - Noflow condition to model rod
  - Weak co-flow air
- Turbulent fluctuations
  - $\ell_t = 3.5mm$, $u' = 0.18m/sec$
  - Estimated $\eta = 220\mu m$

Simulate non-reacting flow in nozzle

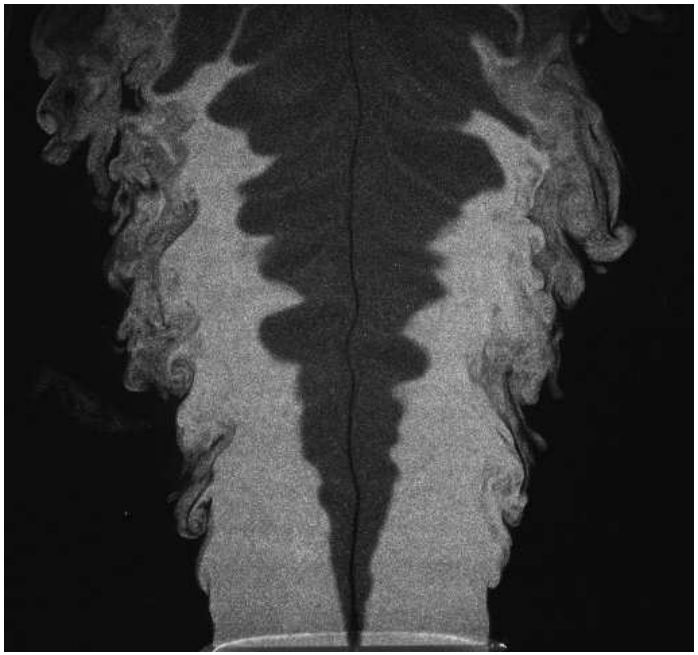
Low Mach number inflow boundary

- Direct coupling to nozzle solver
- Store nozzle outflow data
- Use statistics

# Results: Computation vs. Experiment

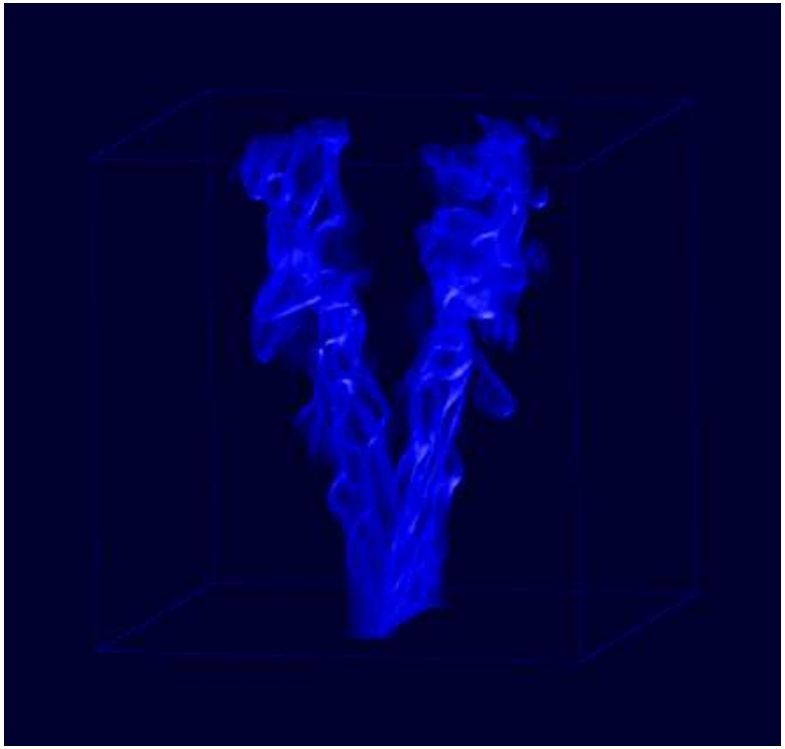



$CH_4$ from simulation

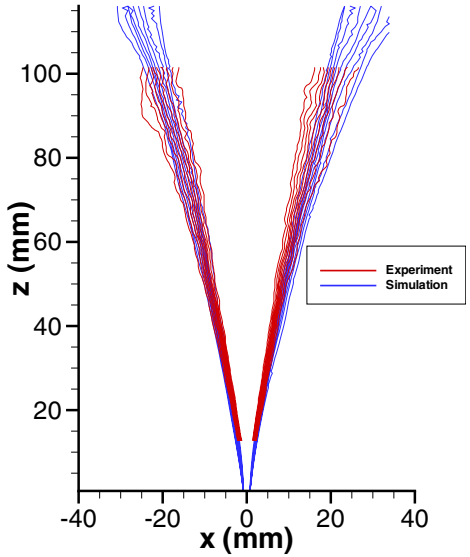


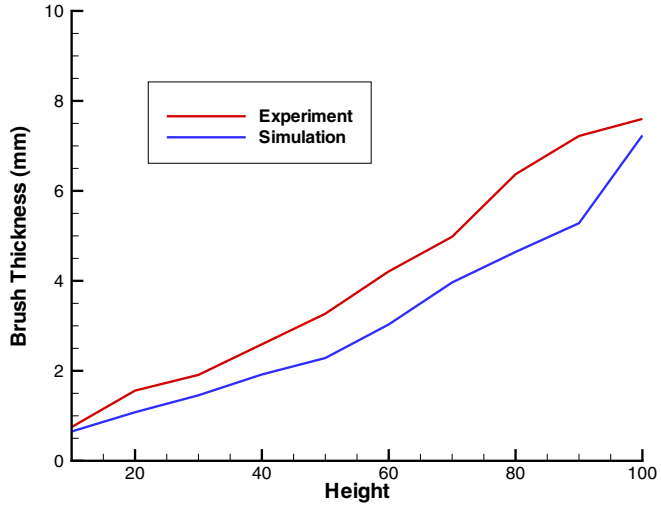
Single image from experimental PIV

# Flame Surface

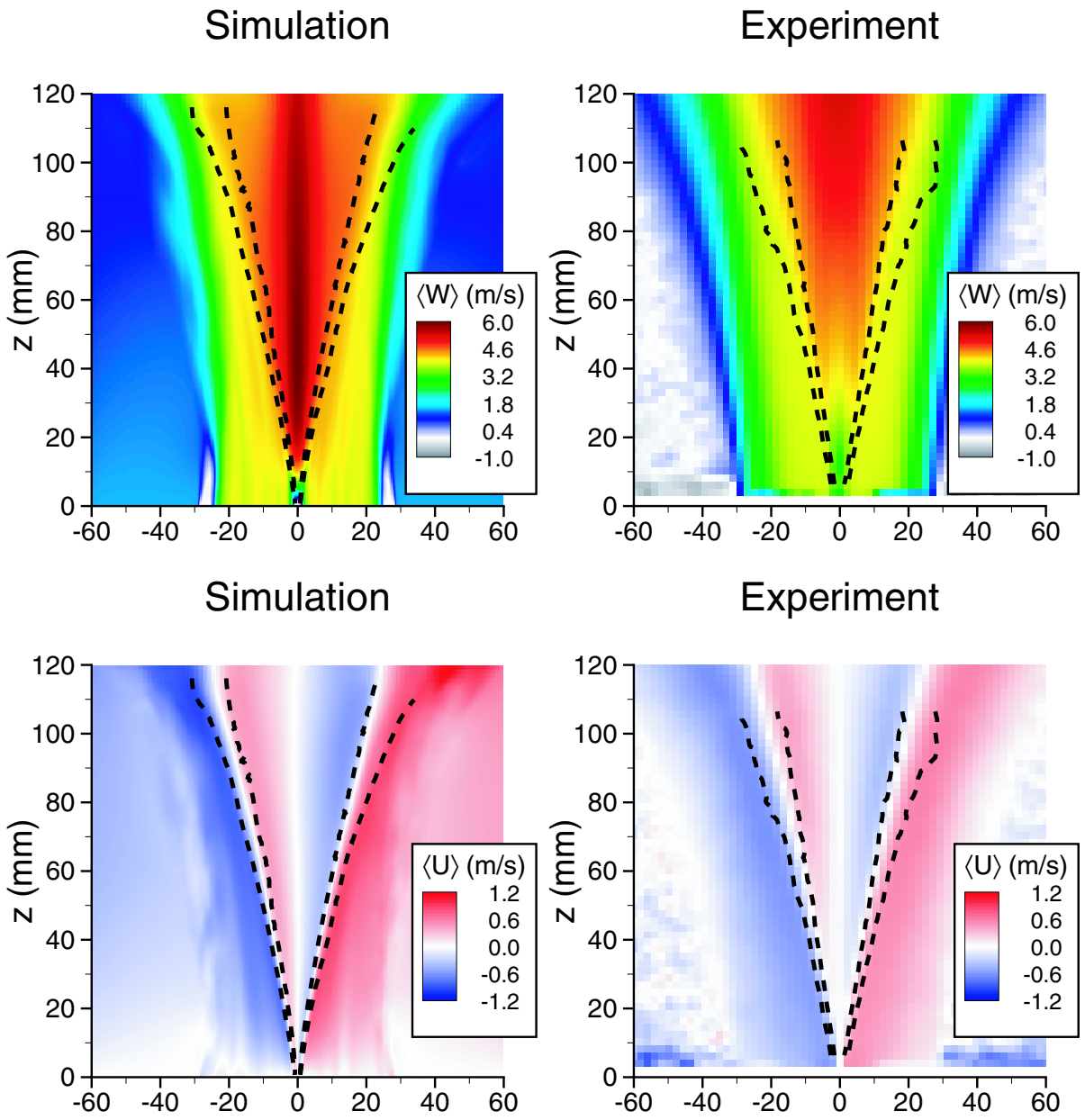


Instantaneous flame surface

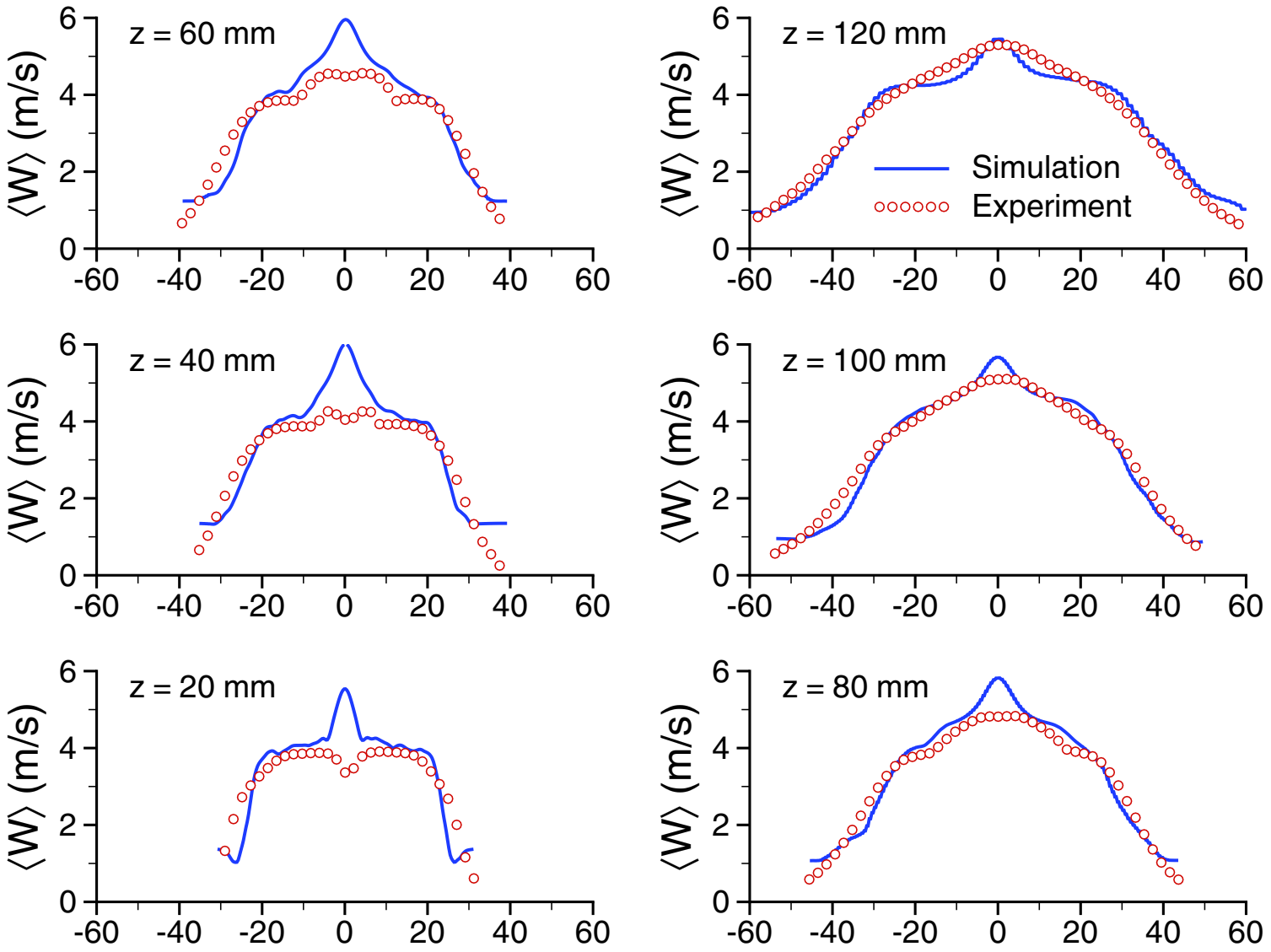


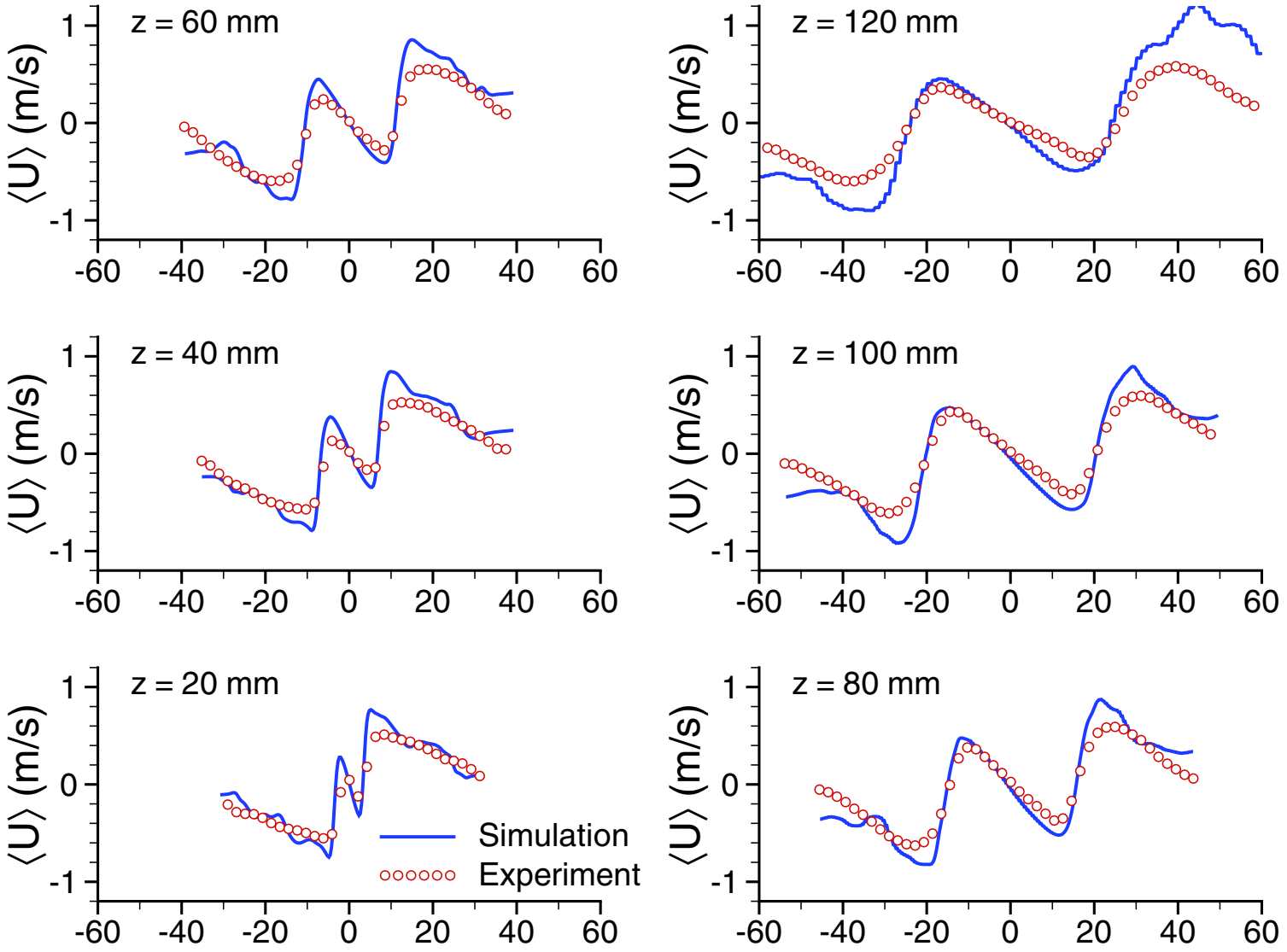
# Velocity comparisons



# Velocity slices – W

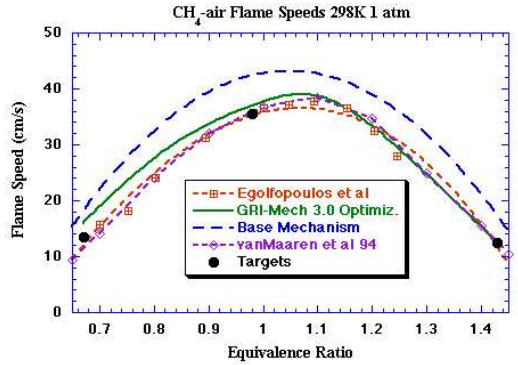


# Velocity slices – U



# Sources of Error

1. Model assumptions, discretization errors
2. Inflow characterization
3. “Laboratory environment” of an unconfined flame
4. Input databases (and parameterizations) for chemical kinetics, thermodynamics, multi-species transport
5. Data extraction from experimental observation, line-of-sight, plane-projected 3D fields, signal modification (PLIF quenching)




The simulation is a sum of weighted judgements and pain threshholds.

Moreover, it is an *iterative* interaction with experimentalists.

- Design experiments with simulation in mind
- Change the traditional experimental paradigm of observe/parametrize/report

# Summary and Future Work

Simulation methodology for turbulent premixed flames

- Low Mach number formulation
- Adaptive
- Conservative
- Second-order in time and space
- Parallel

Laboratory-scale 3D turublent premixed flame – experimental comparisons

- Instantaneous flame wrinkling
- Flame brush statistics
- Velocity statistics

**Future Work**

- Further validation / comparison with experiment
- Modeling of other burners – effect of stabilization
- Characterize turbulent flame propagation properties
- Investigate turbulent flame chemistry